

=> d his

(FILE 'HOME' ENTERED AT 14:46:40 ON 21 MAR 2007)

FILE 'REGISTRY' ENTERED AT 14:46:51 ON 21 MAR 2007

L1 STRUCTURE UPLOADED

L2 3 S L1

L3 28 S L1 SSS FULL

FILE 'CAPLUS' ENTERED AT 14:48:19 ON 21 MAR 2007

L4 1 S L3

FILE 'USPATFULL' ENTERED AT 14:48:46 ON 21 MAR 2007

L5 1 S L3

=> file registry
COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
0.21	0.21

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 14:46:51 ON 21 MAR 2007
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Property values tagged with IC are from the ZIC/VINITI data file
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STRUCTURE FILE UPDATES: 19 MAR 2007 HIGHEST RN 927525-36-8
DICTIONARY FILE UPDATES: 19 MAR 2007 HIGHEST RN 927525-36-8

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

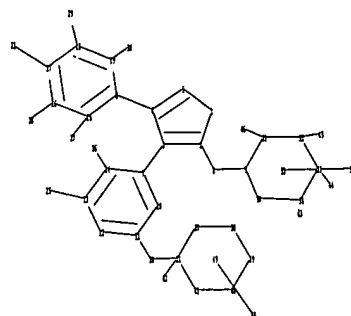
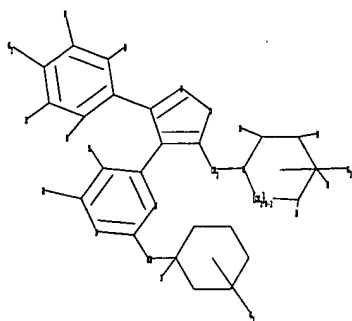
Please note that search-term pricing does apply when
conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10657811final.str



```

chain nodes :
8  20  22  25  26  27  28  29  30  36  42  43  44  45  46  48
ring nodes :
1  2  3  4  5  6  7  9  10  11  12  13  14  15  16  17  18  19  21  31  32  33  34
37  38  39  40  41  50
chain bonds :
2-8  3-7  4-6  8-9  11-20  13-25  14-26  15-27  16-28  17-22  18-29  19-30  20-21
21-42  31-46  32-45  33-44  34-43
ring bonds :
1-2  1-5  2-3  3-4  4-5  6-15  6-19  7-10  7-14  9-31  9-50  10-11  11-12  12-13
13-14  15-16  16-17  17-18  18-19  21-37  21-41  31-32  32-33  33-34  34-50  37-38
38-39  39-40
40-41
exact/norm bonds :
4-5  11-20  17-22  20-21  21-37  21-41  34-50  37-38  38-39  39-40  40-41
exact bonds :
1-2  1-5  2-3  2-8  3-4  3-7  4-6  8-9  9-31  9-50  13-25  14-26  15-27  16-28
18-29
19-30  21-42  31-32  31-46  32-33  32-45  33-34  33-44  34-43
normalized bonds :
6-15  6-19  7-10  7-14  10-11  11-12  12-13  13-14  15-16  16-17  17-18  18-19
isolated ring systems :

```

containing 1 : 6 : 7 : 9 :

G1:H,F

G2:H,O,CH3,CH2,CH

G3:H,CH3,CH2,CH,t-Bu,OH

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:CLASS 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:CLASS 21:Atom
22:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS 31:Atom
32:Atom 33:Atom
34:Atom 36:CLASS 37:Atom 38:Atom 39:Atom 40:Atom 41:Atom 42:CLASS 43:CLASS
44:CLASS 45:CLASS
46:CLASS 48:CLASS 49:Atom 50:Atom 53:Atom

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 14:47:15 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 3 TO ITERATE

100.0% PROCESSED 3 ITERATIONS

3 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 3 TO 163

PROJECTED ANSWERS: 3 TO 163

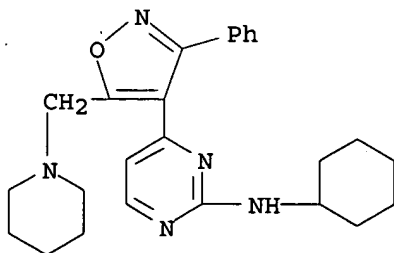
L2 3 SEA SSS SAM L1

=> d l2 scan

L2 3 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 2-Pyrimidinamine, N-cyclohexyl-4-[3-phenyl-5-(1-piperidinylmethyl)-4-
isoxazolyl]- (9CI)

MF C25 H31 N5 O

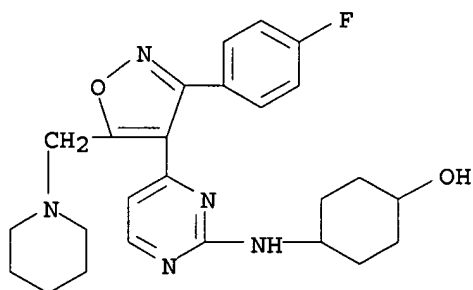


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

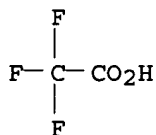
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

L2 3 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN Cyclohexanol, 4-[[4-[3-(4-fluorophenyl)-5-(1-piperidinylmethyl)-4-isoxazolyl]-2-pyrimidinyl]amino]-, mono(trifluoroacetate) (salt) (9CI)
MF C25 H30 F N5 O2 . C2 H F3 O2

CM 1

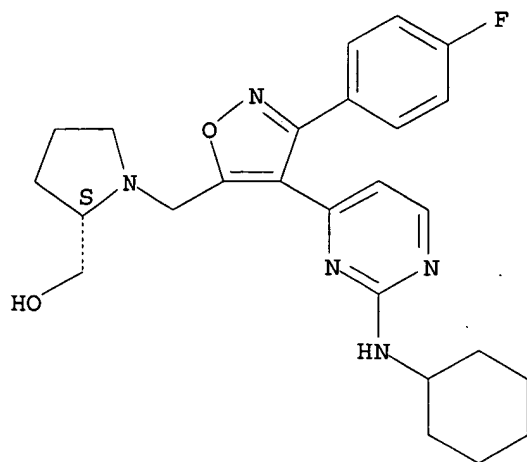


CM 2



L2 3 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN 2-Pyrrolidinemethanol, 1-[[4-[2-(cyclohexylamino)-4-pyrimidinyl]-3-(4-fluorophenyl)-5-isoxazolyl]methyl]-, (2S)- (9CI)
MF C25 H30 F N5 O2

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

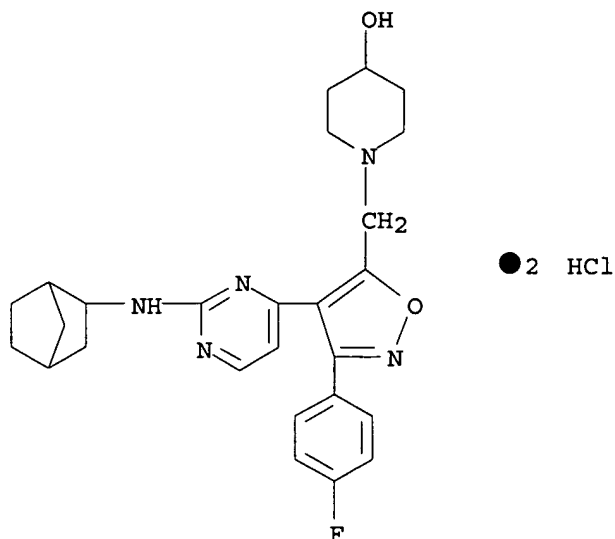
=> s l1 sss full
 FULL SEARCH INITIATED 14:47:50 FILE 'REGISTRY'
 FULL SCREEN SEARCH COMPLETED - 39 TO ITERATE

100.0% PROCESSED 39 ITERATIONS 28 ANSWERS
 SEARCH TIME: 00.00.01

L3 28 SEA SSS FUL L1

=> d l3

L3 ANSWER 1 OF 28 REGISTRY COPYRIGHT 2007 ACS on STN
 RN 673451-61-1 REGISTRY
 ED Entered STN: 09 Apr 2004
 CN 4-Piperidinol, 1-[[4-[2-(bicyclo[2.2.1]hept-2-ylamino)-4-pyrimidinyl]-3-(4-fluorophenyl)-5-isoxazolyl)methyl]-, dihydrochloride (9CI) (CA INDEX NAME)
 MF C26 H30 F N5 O2 . 2 Cl H
 SR CA
 LC STN Files: CA, CAPLUS, USPATFULL
 CRN (673451-55-3)



1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> l d3 scan

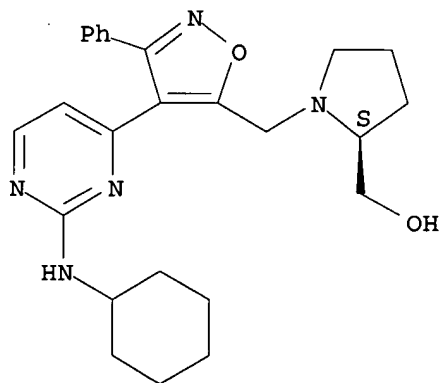
L IS NOT A RECOGNIZED COMMAND

The previous command name entered was not recognized by the system.
For a list of commands available to you in the current file, enter
"HELP COMMANDS" at an arrow prompt (=>).

=> d l3 scan

L3 28 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN 2-Pyrrolidinemethanol, 1-[[4-[2-(cyclohexylamino)-4-pyrimidinyl]-3-phenyl-5-isoxazolyl]methyl]-, (2S)- (9CI)
MF C25 H31 N5 O2

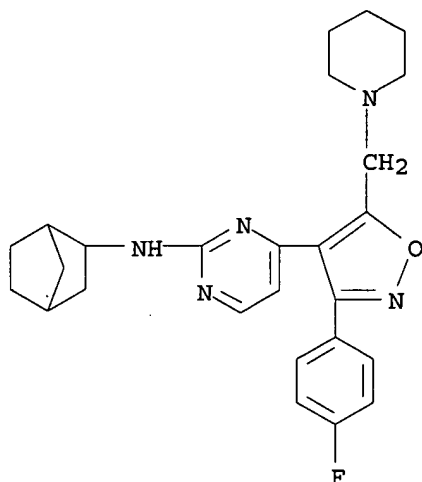
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

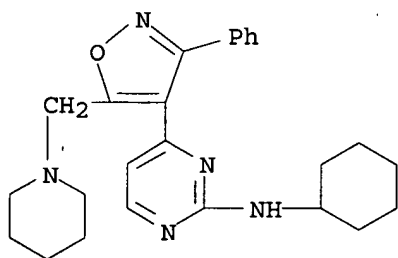
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):4

L3 28 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
 IN 2-Pyrimidinamine, N-bicyclo[2.2.1]hept-2-yl-4-[3-(4-fluorophenyl)-5-(1-piperidinylmethyl)-4-isoxazolyl]- (9CI)
 MF C26 H30 F N5 O



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

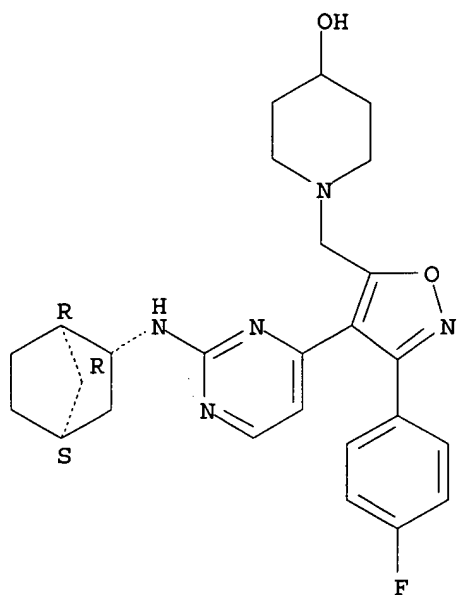
L3 28 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
 IN 2-Pyrimidinamine, N-cyclohexyl-4-[3-phenyl-5-(1-piperidinylmethyl)-4-isoxazolyl]- (9CI)
 MF C25 H31 N5 O



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

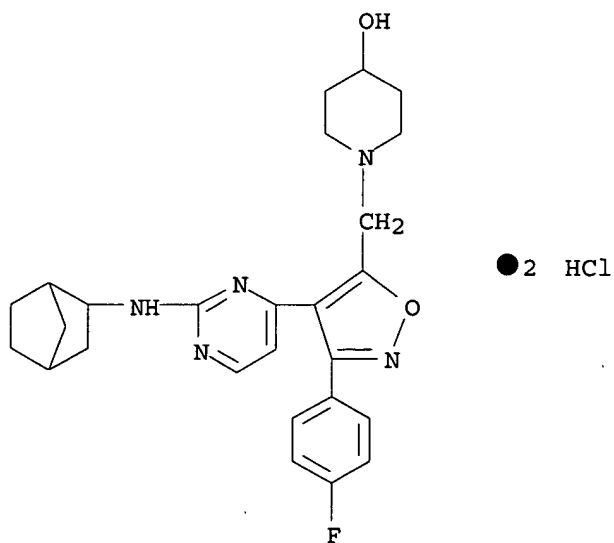
L3 28 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
 IN 4-Piperidinol, 1-[[4-[2-[(1R,2R,4S)-bicyclo[2.2.1]hept-2-ylamino]-4-pyrimidinyl]-3-(4-fluorophenyl)-5-isoxazolyl]methyl]- (9CI)
 MF C26 H30 F N5 O2
 CI COM

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 28 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
 IN 4-Piperidinol, 1-[[4-[2-(bicyclo[2.2.1]hept-2-ylamino)-4-pyrimidinyl]-3-(4-fluorophenyl)-5-isoxazolyl]methyl]-, dihydrochloride (9CI)
 MF C26 H30 F N5 O2 . 2 Cl H



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> file caplus
 COST IN U.S. DOLLARS

SINCE FILE TOTAL
 ENTRY SESSION

FULL ESTIMATED COST

174.50

174.71

FILE 'CAPLUS' ENTERED AT 14:48:19 ON 21 MAR 2007
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FILE COVERS 1907 - 21 Mar 2007 VOL 146 ISS 13
FILE LAST UPDATED: 20 Mar 2007 (20070320/ED)

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=> s l3

L4 1 L3

=> d l4 ti abs bib

L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN
TI Preparation of isoxazoles and their use in the treatment of ischemic diseases
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. I [R1 = H or halo; R2 = (un)substituted cycloalkyl; R3 for each occurrence independently = halo, alkyl, hydroxyalkyl, alkoxyalkyl, etc.; m = 0-2; n = 0-2] and their pharmaceutically acceptable salts are prepared and disclosed as useful for the treatment of neurol., neurodegenerative, ischemic and inflammatory disorders. Thus, e.g., II was prepared in 95% yield via substitution of 3-(4-fluorophenyl)-4-(3-methylsulfonylpyrimidin-4-yl)-5-(4-hydroxypiperidin-1-ylmethyl)isoxazole (preparation given) with cyclohexylamine. Preferred compds. of the invention demonstrated a protection value of $\geq 50\%$ in in vitro ischemia assay. Addnl., compds. were evaluated in in vitro CNS inflammation assays and preferred compds. possessed IC50 values of 300 nM or less. Accordingly, the invention also provides pharmaceutically acceptable compns. comprising the compds. of the invention and methods of utilizing those compds. and compns. in the treatment of neurol., neurodegenerative, ischemic and inflammatory disorders.

AN 2004:220330 CAPLUS <<LOGINID::20070321>>

DN 140:270843

TI Preparation of isoxazoles and their use in the treatment of ischemic diseases

IN Ledebuer, Mark; Ledford, Brian; Maltais, Francois

PA Vertex Pharmaceuticals Incorporated, USA

SO PCT Int. Appl., 46 pp.

CODEN: PIXXD2

DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004022555	A1	20040318	WO 2003-US27903	20030908
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	AU 2003270350	A1	20040329	AU 2003-270350	20030908
	US 2004132755	A1	20040708	US 2003-657811	20030908
	EP 1546141	A1	20050629	EP 2003-752038	20030908
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
	JP 2006502168	T	20060119	JP 2004-534669	20030908
PRAI	US 2002-408813P	P	20020906		
	WO 2003-US27903	W	20030908		
OS	MARPAT 140:270843				
RE.CNT 2	THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD				
	ALL CITATIONS AVAILABLE IN THE RE FORMAT				

=> file uspatfull
COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
3.30	178.01

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
-0.78	-0.78

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FILE 'USPATFULL' ENTERED AT 14:48:46 ON 21 MAR 2007
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FILE COVERS 1971 TO PATENT PUBLICATION DATE: 20 Mar 2007 (20070320/PD)
FILE LAST UPDATED: 20 Mar 2007 (20070320/ED)
HIGHEST GRANTED PATENT NUMBER: US7194769
HIGHEST APPLICATION PUBLICATION NUMBER: US2007061936
CA INDEXING IS CURRENT THROUGH 20 Mar 2007 (20070320/UPCA)
ISSUE CLASS FIELDS (/INCL) CURRENT THROUGH: 20 Mar 2007 (20070320/PD)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Oct 2006
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Oct 2006

=> s l3
L5 1 L3

=> d l5 ti abs bib

L5 ANSWER 1 OF 1 USPATFULL on STN

TI Isoxazoles and uses thereof

AB The present invention provides a compound of formula I: ##STR1##

or a pharmaceutically acceptable salt thereof. These compounds are useful for the treatment of neurological, neurodegenerative, ischemic and inflammatory disorders. Accordingly, the invention also provides pharmaceutically acceptable compositions comprising the compounds of the

invention and methods of utilizing those compounds and compositions in the treatment of neurological, neurodegenerative, ischemic and inflammatory disorders.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AN 2004:172591 USPATFULL <<LOGINID::20070321>>

TI Isoxazoles and uses thereof

IN Ledebor, Mark, Acton, MA, UNITED STATES

Ledford, Brian, Attleboro, MA, UNITED STATES

Salituro, Francesco G., Marlboro, MA, UNITED STATES

PI US 2004132755 A1 20040708

AI US 2003-657811 A1 20030908 (10)

PRAI US 2002-408813P 20020906 (60)

DT Utility

FS APPLICATION

LREP VERTEX PHARMACEUTICALS INC., 130 WAVERLY STREET, CAMBRIDGE, MA,
02139-4242

CLMN Number of Claims: 23

ECL Exemplary Claim: 1

DRWN No Drawings

LN.CNT 1290

CAS INDEXING IS AVAILABLE FOR THIS PATENT.